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DIFFUSION DRIFT PATHS AROUND A $\langle 100 \rangle$ EDGE DISLOCATION IN γ -Fe

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The positions of the atoms around a $\langle 100 \rangle$ edge dislocation in γ -Fe are calculated, using the Johnson-I potential. The boundary conditions were based on isotropic as well as on anisotropic elasticity. The carbon-iron potential, developed by Johnson, was used to calculate paths of maximum energy gain between octahedral sites. Three rows of sinks are found, in regions where the shear stress (2) and the dilatational stress predominate.

COTTRELL and Bilby¹ presented an approximative model for the diffusion of impurity atoms around an isolated edge dislocation. Their model predicts circular drift paths for the impurity atoms from the side of the dislocation where compressional stresses predominate toward the side of predominating dilatational stress. The matrix and the impurity were treated as classical elastic media (continuous and isotropic). Because of the importance of diffusion drift paths for theories concerning the Portevin–Le Châtelier effect (interaction of dislocations with mobile interstitial impurities), we investigated the diffusion of carbon, disregarding the random component of diffusion, by means of computer simulations of a dislocation and impurity on the basis of assumed atomic interaction functions.

For this investigation, we choose a block of γ -Fe, containing about 3500 atoms, which is embedded in an elastic continuum. Because of the low periodicity of the planes along the dislocation line, the edge dislocation with $\langle 100 \rangle$ Burgersvector was chosen. The edge dislocation is introduced in the block using the method of Cotterill and Doyama.² To speed up the relaxation process, the atoms are initially placed in positions as given by elasticity theory; we considered both isotropic and anisotropic elasticity.

Choosing the cartesian coordinate x parallel to

the Burgersvector b , z parallel to the dislocation line, y parallel to the extra half plane, the displacements of the atoms are given in case of isotropic elasticity by:³

$$u_x = \frac{b}{2\pi} \left\{ \arctan\left(\frac{y}{x}\right) + \frac{xy}{2(1-\nu)(x^2+y^2)} \right\} \quad (1)$$

$$u_y = -\frac{b}{2\pi} \left\{ \frac{1-2\nu}{4(1-\nu)} \ln(x^2+y^2) + \frac{x^2-y^2}{4(1-\nu)(x^2+y^2)} \right\} \quad (2)$$

in which ν is the Poisson ratio. The displacements according to anisotropic elasticity are given by:⁴

$$u_x = \frac{b}{4\pi} \left\{ \arctan\left(\frac{2xyA}{x^2-y^2}\right) + B \ln \left(\frac{x^2+y^2+2xyC}{x^2+y^2-2xyC} \right) \right\} \quad (3)$$

$$u_y = -\frac{b}{4\pi} \left\{ D \ln [(x^2+y^2)^2 - 4x^2y^2C^2] - E \arctan \left(\frac{y^2F}{x^2-y^2G} \right) \right\} \quad (4)$$

where C_{11} , C_{12} , C_{44} are the elastic constants and:

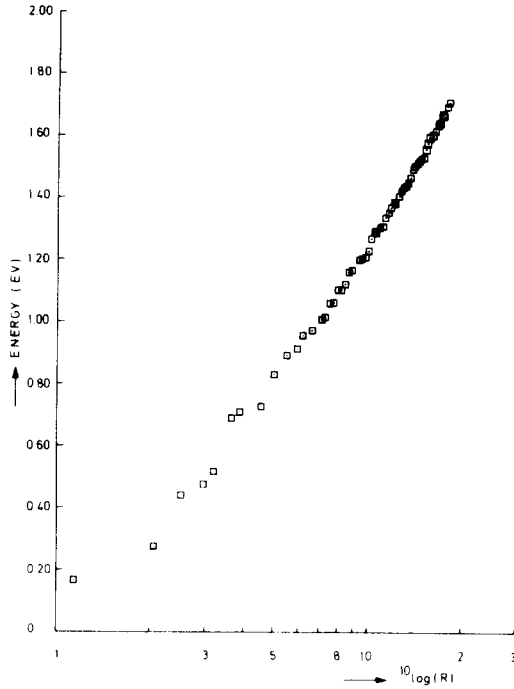


FIG. 1. Energy for one atomic plane within a given radius (\AA) as a function of that radius as measured from the center of the $\langle 100 \rangle$ edge dislocation in γ -Fe.

$$A = \frac{1}{2} \{ (C_{11} + C_{12} + 2C_{44})(C_{11} - C_{12}) / C_{11}C_{44} \}^{\frac{1}{2}} \quad (5)$$

$$B = \frac{1}{2} \{ (C_{11}^2 - C_{12}^2) / (C_{11} + C_{12} + 2C_{44}) \times (C_{12} - C_{11} + 2C_{44}) \}^{\frac{1}{2}} \quad (6)$$

$$C = \frac{1}{2} \{ (C_{12} - C_{11} + 2C_{44})(C_{11} + C_{12}) / C_{11}C_{44} \}^{\frac{1}{2}} \quad (7)$$

$$D = \frac{1}{2} \{ C_{44}(C_{11} - C_{12}) / C_{11}(C_{11} + C_{12} + 2C_{44}) \}^{\frac{1}{2}} \quad (8)$$

$$E = \{ C_{44}(C_{11} + C_{12}) / C_{11}(C_{12} - C_{11} + 2C_{44}) \}^{\frac{1}{2}} \quad (9)$$

$$F = (2C_{11}C_{44})^{-1} \{ (C_{11}^2 - C_{12}^2)(C_{11} + C_{12} + 2C_{44}) \times (C_{12} - C_{11} + 2C_{44}) \}^{\frac{1}{2}} \quad (10)$$

$$G = \{ (C_{11} + C_{12})(C_{12} - C_{11} + 2C_{44}) / 2C_{11}C_{44} \} - 1. \quad (11)$$

The displacements in the z direction are taken to be zero.

The atoms are then permitted to relax to their final positions under influence of the pairwise interatomic interaction function. Using Gibson's⁵ integration procedure, we determine the atomic configuration. In the calculation of the complete dislocation, the atoms are not permitted to relax in the direction parallel to the dislocation line. It is possible to cal-

culate with the integration procedure the atomic configuration which possesses minimum potential energy. We terminated the relaxation process when the energy changes were no more than 5×10^{-4} eV.

A check on the atomic configuration of the edge dislocation can be carried out by calculating the strain energy associated with a dislocation. The energy per unit length along the axis of a cylinder of radius r around the dislocation is given by:

$$E(r) = K \ln \left(\frac{r}{r_c} \right) + E_{\text{core}}. \quad (12)$$

The core energy can be described by:

$$E_{\text{core}} = K \ln \left(\frac{r_c}{r_{eh}} \right) \quad (13)$$

where r_c and r_{eh} represent the core radius and the "equivalent hole radius", respectively. Equation (12) becomes with equation (13):

$$E(r) = K \ln \left(\frac{r}{r_{eh}} \right). \quad (14)$$

In the case of anisotropic elasticity K is given by:

$$K = \frac{b^2}{4\pi} (C_{11} + C_{12}) \{ C_{44}(C_{11} - C_{12}) / [C_{11}(C_{11} + C_{12} + 2C_{44})] \}^{\frac{1}{2}} \quad (15)$$

Figure 1 shows the dislocation energy vs the distance $10 \log r$ from the dislocation line for one plane. Where the curve deviates appreciably from a straight line, we find E_{core} and r_c , while the point of intersection of the straight line on the $10 \log r$ axis provides r_{eh} . We found for r_c 8–9 \AA , r_{eh} 2.3–2.6 \AA and for the core energy 1.1–1.2 eV, which is in accordance with the estimates given by Huntington.⁶ The agreement is reasonable between the calculated value with equation (15) 0.73 eV and the observed value for K in Fig. 1. 0.75–0.8 eV.

The interatomic potential function for iron, developed by Johnson⁷ and the interaction function for carbon–iron,⁸ were used.

In the relaxed crystal block, the potential energy of a carbon atom, placed at an octahedral site was calculated. Each of the octahedral sites was chosen as a starting point of a diffusion path. Except in the follow-

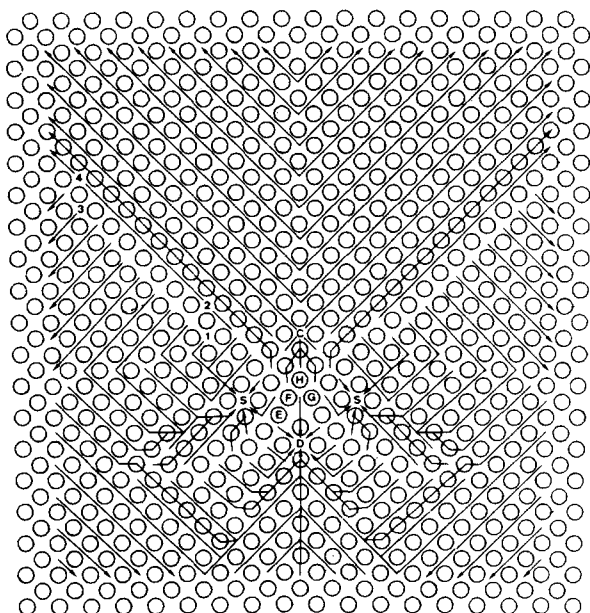


FIG. 2. Diffusion paths diagram of a carbon interstitial around a $\langle 100 \rangle$ edge dislocation in γ -Fe. The sites numbered D and S represent the minima which were found with isotropic boundary conditions.

Table 1. The effect of the choice of the boundary conditions on the strains (per cent) in the core region of a $\langle 100 \rangle$ edge dislocation in γ -Fe. For the numbering of the atoms, see Fig. 2

Bonding	Isotropy	Anisotropy
E-F	- 8.861	- 8.840
F-G	- 25.377	- 25.391
F-H	- 2.592	- 2.601

ing special cases the lattice with a carbon atom at the sinks which were found, at the secondary minima and in the neighbouring sites around the sinks. In the case of boundary conditions based on isotropic elasticity (Fig. 2), we found three minima; two in the region where shear stress predominates (S) and one in the region with dilatational stress (D). If the boundary conditions were chosen according to anisotropic elasticity, only one minimum D and three secondary minima were found. The secondary minima C and $S(2)$ disappeared after relaxing the lattice anew (Fig. 3).

The effect of the boundary conditions is less pronounced for the strains and the bond lengths in the model. Three strains in the core region are listed in Table 1 in the case of isotropic and anisotropic

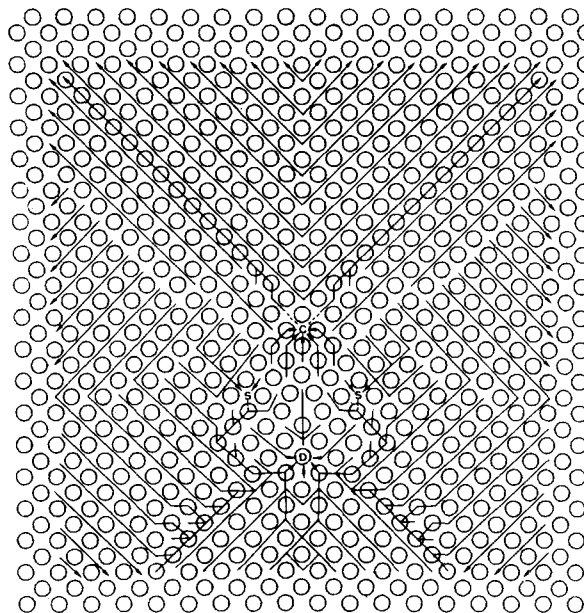


FIG. 3. Diffusion paths diagram of a carbon interstitial around a $\langle 100 \rangle$ edge dislocation in γ -Fe, where the boundary conditions have been given by anisotropic elasticity. Of the indicated minima C , S , D , only D remains; after relaxing the lattice anew with the carbon placed at S , C , respectively, and their neighbouring sites, these minima disappear.

boundary conditions. The effect on the diffusion drift paths can be larger because they are sometimes determined by energy differences of the order of magnitude of $10^{-3} - 10^{-4}$ eV.

The influence of the block size was also investigated. A previous calculation⁹ of diffusion drift paths in a crystal block containing 10 planes of 200 atoms, shows two sinks S , one sink D and also one minimum in the compressional region C . The minima D and S are situated at the same place in the small model as in the present model. In the small model we also calculated the diffusion drift paths choosing the octahedral sites on the plane above the figures as starting points. The minimum C at the compressional side (Fig. 2) disappears in the larger model because the boundary effects are eliminated. Furthermore, the diffusion path as given in Fig. 2 and Fig. 3 are based on the lattice with unrelaxed positions for the carbon atoms. The checks we made by relaxing anew with an interstitial at several consecutive positions along the diffusion path, did not indicate that the diffusion paths would have been considerably different from those calculated from the unrelaxed positions.

Table 2. The potential energies for one carbon atom (E_I) placed at the sinks of the diffusion paths S and D. ΔE_{ID} represents the difference between the configurational energy of the relaxed lattice containing a $\langle 100 \rangle$ edge dislocation in γ -Fe and the configurational energy of the lattice, when it is relaxed anew with one carbon at the sinks S and D

Energy (eV)	Isotropy		Anisotropy	
	$-E_I$	$-\Delta E_{ID}$	$-E_I$	$-\Delta E_{ID}$
Site S	0.983	1.933	0.980	1.940
D	0.997	1.975	0.996	1.969

The potential energies for the carbon atoms placed at the sites D and S, are listed in Table 2. We suspect that the storage capacity for carbon atoms will be considerable because of the shallowness of the minima D and S.

Our calculation of the diffusion gradients and the diffusion drift paths differ mainly from those predicted by the theory of Cottrell and Bilby inside the core region. At a distance of about 5 Burgersvectors from the dislocation line, the calculated drift paths approximate the circular shapes predicted by the Cottrell-Bilby theory except in the compressional region, around which a boundary appears. The height of the boundary

reduces with increasing distance from the dislocation core. An indication for the height of the boundary is the energy difference for a carbon atom placed at octahedral sites on both sides of the boundary (sites 1,2 and 3,4 in Fig. 2). This energy difference reduces from $\Delta E_{1,2} = 0.003$ eV to $\Delta E_{3,4} = 0.0003$ eV. Bearing in mind that the lattice is relaxed till the potential energy difference is less than 5×10^{-4} eV and that we neglected the random diffusion component, it is evident that the interstitial atom can easily cross the boundary at a distance of about $5b\sqrt{2}$ from the dislocation core.

In a subsequent paper the diffusion gradients for a carbon interstitial within a $\frac{1}{2}\langle 111 \rangle (110)$ slipsystem in α -Fe shall be presented.

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